Stripes, pseudogaps, and SO(6) in the cuprate superconductors

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We briefly summarize two related calculations. First, we demonstrate that the instabilities (either nesting or pairing) associated with the high-T$_c$ cuprates can be described by an $SO(6)$ transformation group. There are two independent 6-dimensional representations ('superspins'). One superspin combines Zhang's 5-component superspin with a flux phase instability; the other involves a charge density wave, s-wave superconductivity, and an exotic spin current.

The second calculation is a self-consistent slave boson calculation, which provides a good description of the doping dependence of the photoemission dispersion in terms of dynamic striped phases. The stripes are stabilized by strong electron-phonon coupling, and provide evidence for a doping-dependent crossover between the two superspin groundstates.

I. $SO(6)$ INSTABILITY GROUP

$i\eta_-$				
Π_{x+}	$-A_x$			
Π_{y+}	$-A_y$	$-S_z$		
Π_{z+}	$-A_z$	S_y	$-S_x$	
Q	η_+	$-i\Pi_{x-}$	$-i\Pi_{y-}$	$-i\Pi_{z-}$

FIG. 1. Matrix Representation of SO(6), using the shorthand $O_\pm = O \pm O^\dagger$.

Zhang [1] has proposed that the physics of doping the cuprate superconductors is controlled by an $SO(5)$ transformation group, having a 5-dimensional superspin representation which mixes spin-density wave (SDW) and d-wave superconducting components. This is in contradiction to earlier findings [2] that in the Hubbard model at half filling d-wave superconductivity is symmetry-equivalent to a flux phase [3]. Here, we show that Zhang's $SO(5)$ group is a subgroup of an $SO(6)$ group, the instability group of the two-dimensional (2D) Van Hove singularity (VHS) [4]. The corresponding 6-component superspin combines Zhang's superspin with a flux-phase instability.

Consider an electronic state with a two-fold orbital degeneracy, ψ_1, ψ_2. Including spin and charge conjugation,

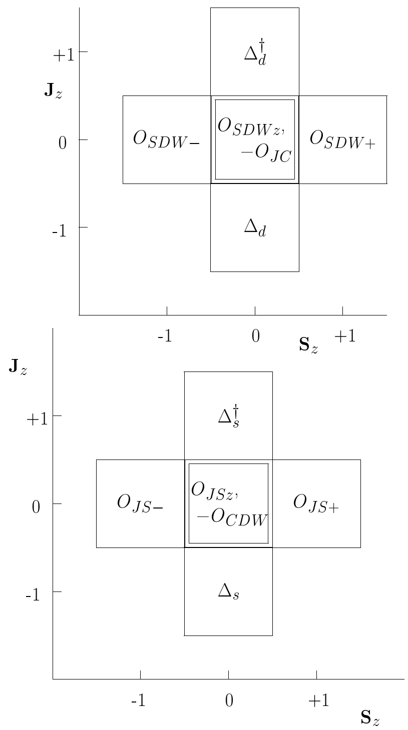

FIG. 2. $SO(4)$ weight diagram of $\mathbf{V}_s$ (top) and $\mathbf{V}_h$ (bottom), where S_z (J_z) is the z component of spin (pseudospin).

8 single particle operators can be formed, or $8\times 7/2 = 28$ pair operators (taking account of the Pauli exclusion principle). These operators can be combined into a representation of an $SO(8)$ group, the pair group [4] which controls the various pairing and nesting instabilities which can arise. For the quasi-2D cuprates, the orbital degeneracy is associated with the VHS's along $(\pi,0)$ and $(0,\pi)$; because of the large density of states (dos) at a VHS, the Fermi surface can be approximated by just two points [5,6], similar to a one-dimensional metal.

Consider a supercell of size $2a\times 2a$, each cell containing four atoms. Let $\vec{i}$ be a lattice vector of the original lattice, and $\vec{r}$ be a lattice vector of the supercell lattice. If the Cu-site operators are a's, then the VHS operators are

$$\psi_{1\sigma}(\vec{r}) = \frac{1}{2}(a_{\vec{i},\sigma} - a_{\vec{i}+\hat{x},\sigma} + a_{\vec{i}+\hat{y},\sigma} - a_{\vec{i}+\hat{x}+\hat{y},\sigma})$$
$$\psi_{2\sigma}(\vec{r}) = \frac{1}{2}(a_{\vec{i},\sigma} + a_{\vec{i}+\hat{x},\sigma} - a_{\vec{i}+\hat{y},\sigma} - a_{\vec{i}+\hat{x}+\hat{y},\sigma}). \qquad (1)$$

(The remaining operators are located in other parts of the Brillouin zone, and play a negligible role in nesting phenomena.)

A special role is played by the operator τ =

$\sum_{\vec{r},\sigma}(\psi^\dagger_{1\sigma}(\vec{r})\psi_{1\sigma}(\vec{r}) - \psi^\dagger_{2\sigma}(\vec{r})\psi_{2\sigma}(\vec{r}))$, which splits the VHS degeneracy. The operators which commute with τ form an $SO(6)$ transformation group, Fig. 1, with two fundamental 6-dimensional representations, Fig. 2. The momentum-space representation of the superspin operators is shown in Table I; the full list is in Ref. [4]. Since the generators of $SO(6)$ can be represented as antisymmetric 6×6 matrices, Fig. 1 assigns each operator to the position of the corresponding non-zero matrix element, to produce the correct $SO(6)$ Lie algebra

$$[L^{ij}, L^{km}] = i(\delta_{ik}L^{jm} + \delta_{jm}L^{ik} - \delta_{im}L^{jk} - \delta_{jk}L^{im}). \tag{2}$$

Note that by deleting the second row and column, an $SO(5)$ subalgebra is generated, which is equivalent to the one postulated by Zhang [1].

In Fig. 2, the pseudospin operator [7] is

$$J_- = 2\eta, \quad J_+ = 2\eta^\dagger, \quad J_z = Q, \tag{3}$$

and $O_{SDW\pm} = \mp(O_{SDWx} \pm iO_{SDWy})/\sqrt{2}$. The superspin $\mathbf{V_s}$ consists of a spin-density wave spin triplet ($\vec{O}_{SDW}$) and a pseudospin triplet combining d-wave superconductivity (Δ_d, $\Delta_d^\dagger$) and an orbital antiferromagnet (O_{JC}) equivalent to the flux phase operator [3]. The superspin $\mathbf{V_h}$ consists of a spin current spin triplet ($\vec{O}_{JS}$) and a charge-density wave (O_{CDW}), s-wave superconductivity (Δ_s, $\Delta_s^\dagger$) pseudospin triplet. These operators are equivalent to those introduced by Schulz [6] and, in a related context, by Halperin and Rice [8].

Table I: Fourier Transforms of Superspins

Operator	Representation
O_{CDW}	$2\Sigma_{\vec{k}\sigma}(a^\dagger_{\vec{k}\sigma}a_{\vec{k}+\vec{Q},\sigma})$
$O_{SDW\alpha}$	$2\Sigma_{\vec{k},i,j}(a^\dagger_{\vec{k},i}\sigma^\alpha_{ij}a_{\vec{k}+\vec{Q},j})$
Δ_s	$2\Sigma_{\vec{k}}(a_{\vec{k}\uparrow}a_{-\vec{k}\downarrow})$
O_{JC}	$-\Sigma_{\vec{k}\sigma}g(\vec{k})(a^\dagger_{\vec{k}\sigma}a_{\vec{k}+\vec{Q},\sigma})$
$O_{JS\alpha}$	$-\Sigma_{\vec{k},i,j}g(\vec{k})(a^\dagger_{\vec{k},i}\sigma^\alpha_{ij}a_{\vec{k}+\vec{Q},j})$
Δ_d	$-\Sigma_{\vec{k}}g(\vec{k})(a_{\vec{k}\uparrow}a_{-\vec{k}\downarrow})$

In weak coupling, the instabilities are controlled by their respective susceptibilities and the form of the quartic interaction terms. For an energy dispersion

$$\epsilon_{\vec{k}} = -2t(\cos k_xa + \cos k_ya) + 4t'\cos k_xa\cos k_ya, \tag{4}$$

then when $t' = 0$ and at exactly half filling (square Fermi surface), the model has an extra pseudospin symmetry [7], and all the bare susceptibilities are equal [4]. The dressed susceptibilities are

$$\chi_i = \frac{\chi_{0i}}{1 + 2\chi_{0i}G_i}, \tag{5}$$

where G_i is related to the quartic coupling. Since all 12 χ_{0i}'s are equal (at half filling), the ground state instability is controlled by the interactions G_i. For a pure Hubbard model, the U term breaks the $SO(6)$ symmetry, leading to a negative G_{SDW} and a positive G_{CDW}, G_s, Fig. 3. Thus at half filling the ground state is antiferromagnetic, O_{SDW}.

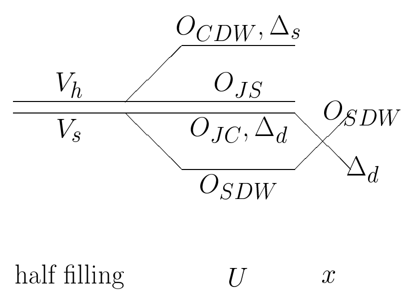

FIG. 3. Splitting of $SO(6)$ superspin degeneracies by interaction U and by doping x.

Doping away from half filling breaks the pseudospin symmetry, leading to two distinct susceptibilities, χ_{00} for the particle-hole operators and χ_{02} for the particle-particle operators, Fig. 4. Since the susceptibilities are enhanced by nesting, their magnitudes fall off with doping. However, the magnitude of χ_{00} falls much more rapidly, leading to a possible scenario for d-wave superconductivity, Fig. 3 [4]: if there is an attractive interaction for d-wave superconductivity, it will be overwhelmed by the strong divergence in χ_{SDW} at half filling, but with doping, the SDW instability falls off much faster, leading to a possible crossover to d-wave superconductivity. This is consistent with earlier renormalization group results [5,9,10].

In a more realistic, strong coupling model, a number of additional features must be considered. First, additional hopping parameters, such as the second-neighbor t' term in Eq. 4, also break the pseudospin degeneracy, Fig. 5. Note that the susceptibility diverges away from half filling, at the VHS, but even at optimal doping $\chi_{02} >> \chi_{00}$. Moreover, by comparing Fig. 4 it can be seen that χ_{02} is actually larger, at optimal doping, for $t' \neq 0$. Since strong coupling pins the Fermi level near the VHS over an extended doping range [11,12], this enhancement of χ_{02} can greatly enhance the possibility for d-wave superconductivity to arise on doping.

There is considerable evidence for phonon coupling and structural instabilities in the doped material [10]. Hence, it is interesting to see whether strong electron-phonon coupling can cause a crossover to a groundstate involving $\mathbf{V}_h$. Since the CDW operator is proportional to the difference in hole population of the odd and even sublattices, it must vanish in the strong coupling limit at

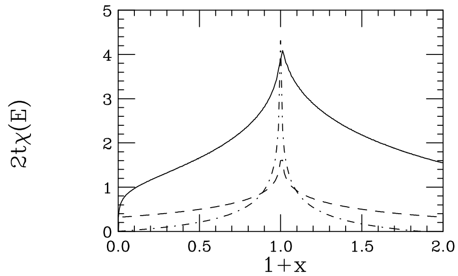

FIG. 4. Susceptibilities χ_{00} (dotdashed line) and χ_{02} (solid line) and density of states (dashed line) vs. band filling $1+x$ for the one band model with $t'=0$.

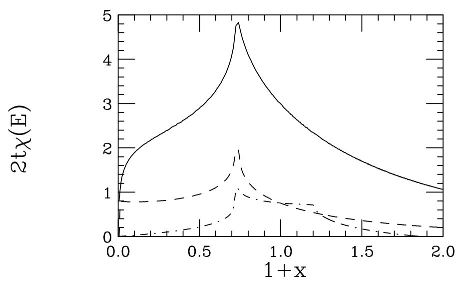

FIG. 5. As in Fig. 4, but with $2t'=-0.3t$.

half filling, when there is one hole per Cu. For finite doping there can be a CDW order, with $< O_{CDW} > \propto x$, if all the holes are confined to one sublattice. The resulting structure is equivalent to that found in $La_{2-x}Sr_xNiO_4$ for $x\sim 0.5$ [13]. Moreover, such a structure is closely related to the holon condensate [14] introduced to overcome parity-violation problems in anyonic models of superconductivity. In these models, two species of holons are introduced, of opposite parity violation. A coherent superposition of the two preserves parity, while producing a *holon condensation*, wherein all holons are confined to one sublattice, leading to a real-space CDW [15].

In the following section, we describe a slave boson calculation [12] which self-consistently takes into account both strong coupling effects and strong electron-phonon coupling. We show that VHS pinning can provide a natural explanation for the observed stripe phases [16,17] in these materials, as well as pseudogaps and extended VHS's.

II. CDW ORDER AND PHASE SEPARATION

In the strong coupling limit, the dominant physics is quite different. At exactly half filling, there is a metal-insulator transition that is unrelated to nesting: a Mott transition, or charge transfer insulator transition in the three-band model of the cuprates which will be employed here. The nesting/pairing instabilities arise on top of this transition, and are strongly constrained by the large Hubbard U, which limits double occupancy of the Cu orbitals. In the slave boson approach employed here, the limit $U\to\infty$ is taken (no double occupancy). To include spin effects, it is necessary to go beyond the standard slave boson approach, either by introducing four slave bosons [18] or by introducing a Heisenberg exchange J [19] – the latter approach is followed here.

Thus, the starting point of the analysis is the three-band model Hamiltonian:

$$H=\sum_{j,\sigma}\Big(\Delta d^\dagger_{j,\sigma}d_{j,\sigma}+\sum_{\hat\delta}t_{CuO}[d^\dagger_{j,\sigma}p_{j+\hat\delta,\sigma}+(c.c.)]$$
$$+\sum_{\hat\delta'}t_{OO}[p^\dagger_{j+\hat\delta,\sigma}p_{j+\hat\delta',\sigma}+(c.c.)]$$
$$+J\sum_{\hat\delta'',\sigma'}d^\dagger_{j,\sigma}d_{j,\sigma'}d^\dagger_{j+\hat\delta,\sigma'}d_{j+\hat\delta,\sigma}\Big). \qquad (6)$$

In this equation, $d^\dagger$ ($p^\dagger$) is a creation operator for holes on Cu (O), j is summed over lattice sites, $\hat\delta$ over Cu-O nearest neighbors, $\hat\delta'$ ($\hat\delta''$) over O-O (Cu-Cu) neighbors, and c.c. stands for complex conjugate. The band parameters are Δ, the splitting between the Cu and O energy levels, t_{CuO}, the Cu-O hopping parameter, t_{OO}, the O-O hopping parameter, and J the exchange constant.

In the above equation, the limit $U\to\infty$ has been taken, and a slave boson introduced to prevent Cu double occupancy. The parameters t_{CuO} and Δ are renormalized values, to be solved self-consistently [12]. In the exchange energy, the d^4-term is decoupled in mean-field as

$$J\sum_{j,\hat\delta'',\sigma,\sigma'}d^\dagger_{j,\sigma}d_{j,\sigma'}d^\dagger_{j+\hat\delta,\sigma'}d_{j+\hat\delta,\sigma}\to$$
$$\frac{2N_s}{J}\Delta_1^2+\sum_{j,\hat\delta'',\sigma}(\Delta_{j,j+\hat\delta''}d^\dagger_{j,\sigma}d_{j+\hat\delta'',\sigma}+c.c.) \qquad (7)$$

where N_s is the number of unit cells and

$$\Delta_{ij}\equiv J\sum_\sigma < d_{i\sigma}d^\dagger_{j\sigma} >=\Delta_1 e^{i\theta_{ij}}. \qquad (8)$$

Depending on the choice of phase, a variety of magnetic states are possible. Here the only choices considered are $\theta_{ij}=0$, corresponding to a uniform phase (only short-range magnetic correlations), and $\theta_{ij}=\pm\pi/4$ for a flux [3] phase, with the $\pm$ sign chosen so that the net phase change around any plaquette is π.

Finally, electron-phonon coupling is included by the substitution $t_{CuO}=t(1\pm\delta)$, with δ due to a CDW distortion: for a breathing mode, all four Cu-O bonds are equivalent for any given Cu, but all are long ($t_{CuO}=t(1-\delta)$) for one sublattice, and short for the other. Note that this model includes only two of the twelve possible superspin components, but already gives rise to a complicated phase diagram. It should describe the $\mathbf{V_s}\to\mathbf{V_h}$ ($O_{JC}\to O_{CDW}$) crossover.

A charge transfer insulator transition is found at half filling when Δ exceeds a critical value [20]. Near half filling, the flux phase is stable, and the CDW is suppressed by strong coupling effects. However, if the electron-phonon coupling is strong enough, there is a crossover in the doped material to a CDW phase, which is maximally stable near the doping at which the Fermi level crosses the bare VHS. As had been previously noted [21], the flux phase provides a good description of the measured energy dispersion in insulating cuprates [22], Fig. 6, while the CDW fits the dispersion near optimum doping [23], in particular reproducing the extended VHS. [Note however that the present calculations underestimate the total dispersion by a factor of 2.]

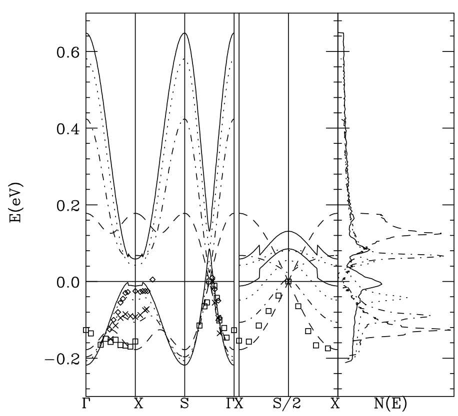

FIG. 6. (a) Energy dispersion for the flux phase at half filling $x_1 = 0^+$ (dashed line) and the paramagnetic phase at $x = 0.22$, $V_{ep} = 0.6$eV (solid line), close to the minimum free energy, and for the fluctuating stripe phase model, for $\nu_c = 0.5$ (dotdashed line) and 0.75 (dotted line). Data from underdoped Bi-2212 (diamonds and $\times$'s) [23] or SCOC (squares) [22] are plotted as E/2. Special points of the Brillouin zone are X = (π,0), S = (π, π). (b) Density of states vs. energy, for the same parameters.

The situation for intermediate dopings is more complex. The free energy minimum at finite doping associated with the CDW leads to an instability toward phase separation between magnetic (flux phase) and charged (CDW) domains. There is considerable experimental evidence for such phase separation in the cuprates [24,25,10], which can be macroscopic if the doping counterions are mobile (e.g., the interstitial oxygen in $La_2CuO_{4+\delta}$ [26]. More commonly, Coulomb repulsion between holes restricts the phase separation to a nanoscopic scale [27], typically forming striped phases [16,17]. The driving mechanism for this phase separation has variously been ascribed to large J [28,29], to the nearest neighbor Coulomb energy V [30], or, as in the present case, to VHS-induced CDW formation [11].

In modeling the striped phase, a static stripe pattern produces too much structure in the dispersion, due to minigaps [31,12]. If a fluctuating striped phase is approximated by taking the weighted average of the end-phase band parameters, good agreement with the experimental dispersion is found, Fig. 6. In this figure $\nu_c = x/x_c$ is the fraction of charged stripes, with x_c the doping of the uniformly doped charged end phase, here taken as $x_c = 0.288$. The same model also describes the crossover from small (hole pockets) to large Fermi surface with doping, Fig. 7.

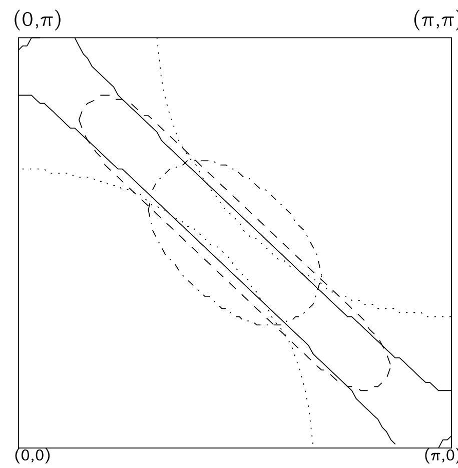

FIG. 7. Fermi surfaces for the fluctuating stripe phase model, for $\nu_c = 1.0$ (dotted line), 0.5486 (solid line), 0.5 (dashed line), and 0.25 (dotdashed line).

A number of points should be made. (1) The splitting of the bands near the X-point, $(\pi, 0)$, provides a good descrpition of pseudogap formation in the cuprates – not only the photoemission data, Fig. 6, but also thermodynamic data from heat capacity and magnetization [32], as well as the temperature-doping phase diagram [33]. The smooth doping dependence masks a crossover from spin-like to charge-like instability – from $\mathbf{V_s} \rightarrow \mathbf{V_h}$. Accordingly, the underdoped results near half filling are in good agreement with recent Monte Carlo calculations [34]. (2) From Fig. 6b, it is clear that the pseudogap is directly associated with the splitting of the VHS degeneracy, and hence with the properties of $SO(6)$. (3) Campuzano [35] reports a different doping dependence of the $(\pi, 0)$ photoemission, namely that there are two independent features, one a sharp quasiparticle peak which is near the Fermi level at optimal doping, and broadens severely in underdoped samples, and the second a broad peak which is already present at ∼200meV below the Fermi level in optimally doped material, and gradually shifts to 300meV with increased underdoping. A dynamic fluctuation model can accomodate this in terms of a dynamic average of the two end phases. (4) There is considerable evidence for short-range CDW order in the doped cuprates, summarized in Ref. [10], Section 9.2, often associated with CuO bond stretching [36]. (5) In the

present model, the pseudogap is associated with magnetic or structural instabilities which compete with superconductivity. Hence, there should be a separate superconducting gap, which scales with T_c and ν_c [33]. This gap may be related to the spin gap and resonance peak seen in neutron scattering measurements of the magnetic susceptibility near $S=(\pi,\pi)$ [37]. (6) In the overdoped regime, the CDW undergoes a quantum phase transition, $T_{CDW}\rightarrow 0$. It has been suggested that such a QCP can lead to high-T_c superconductivity [38].

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